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Michael Danos

U.S. DEPARTMENT OF COMMERCE  
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**U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, *Secretary***  
**NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director***



# IRREDUCIBLE DENSITY MATRICES

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## ABSTRACT

An expansion of the density matrix is given into irreducible  $SU(2)$  tensors, i.e., into quantities of good angular momentum. These irreducible tensors can be handled by all the powerful tools developed in the context of the handling of angular momentum. As examples, the density matrix of a cryogenically aligned nucleus is derived and the construction of the angular distributions of nuclear reactions in terms of density matrices is demonstrated.

Key words: angular distributions; angular momentum; impure quantum states; polarization; quantum theory; reaction theory



## I. INTRODUCTION

As is well known one may express all of quantum mechanics in terms of density matrices. One must use density matrices when dealing with impure states [1].<sup>1</sup> Most prominent among such cases is the description of systems in thermal equilibrium with some heat bath at non-zero temperature. Examples for this are cryogenically aligned or polarized targets for nuclear physics experiments in which angular distributions or polarization, etc., are studied. As has been variously emphasized, such situations are best described in terms of irreducible tensors, i.e., of quantities which undergo certain well-defined transformations under rotations [2]. The aim of this note is to propose conventions for defining irreducible density matrices which are designed to allow the incorporation of these quantities into the angular momentum calculus in as smooth a manner as possible, i.e., in such a way that no superfluous phases appear. In other words, this note aims at extending an earlier paper [3] to include density matrices into a consistent set of definitions. This way they then can be treated by all the powerful tools of Racah calculus including the graphical method introduced in Ref. 3 (see also Ref. 4). We shall employ these techniques in the present note, and refer the reader for a complete description of the notation and the techniques to Chapter 4 of Ref. 5.

In section II the density matrix is introduced in the context of the evaluation of the expectation value of an operator for the case of a pure state. The definition of the irreducible density matrix this way is achieved in a natural way. As examples for the use of density matrices we describe the

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<sup>1</sup>Numbers in brackets indicate the literature references at the end of this document.

construction of the expressions for the angular distributions and polarizations of reactions of arbitrary complexity. It is here that the advantage of using the consistent definitions for the density matrices becomes apparent in that one automatically achieves the complete expressions including the interference terms in a manner which essentially eliminates the possibility of errors, including errors in phasing. The expressions are written in terms of the density matrices of the initial and final states and of the analyzing instruments, and thus are fully general. In this section also the special precautions are mentioned one must observe if one works in the occupation number representation, i.e., if the amplitudes are creation-annihilation operators.

The general case of an impure state is considered in section III where it is shown that all the results of section II, i.e., of the density-matrix formulation for pure states, are immediately applicable in the general case. As an example of an impure state the density matrix of a nucleus in thermal equilibrium with a crystal lattice is derived in full detail. This is done for the case where the lattice field is of arbitrary multipolarity.

The relation of the irreducible density matrix to the density matrix defined in the usual way is demonstrated in section IV. Finally, in the Appendix, some definitions are collected for the convenience of the reader.

## II. PURE STATES

Consider a state of given angular momentum and polarization. It is written as the invariant

$$\psi =: \sum_M a_M^{(I)} \psi_M^{[I]} = \hat{I} [a^{[I]} \psi^{[I]}] [0]$$

$$\hat{I} =: (2I + 1)^{\frac{1}{2}} . \quad (1)$$

We use the usual convention [2-5]

$$a_M^{(I)} =: (-)^{I+M} a_{-M}^{[I]} . \quad (2)$$

Care has to be taken when constructing the "complex conjugate" state if it describes a system containing Fermions. We shall therefore separate the conjugation explicitly into the two components: change of the gender (contrastandard — costandard) and "transpose." We thus write

$$\psi^\dagger = \sum_M a_M^{(I)\dagger} \psi_M^{[I]\dagger} \quad (3)$$

together with the definitions (convention):

$$\psi_M^{[I]\dagger} =: \tilde{\psi}_M^{(I)} = (-)^{I+M} \tilde{\psi}_{-M}^{[I]} \quad (4a)$$

$$\tilde{\psi}_M^{[I]\dagger} = (-)^{2I} \psi_M^{(I)} = (-)^{I-M} \psi_{-M}^{[I]} \quad (4b)$$

and, similarly for the amplitudes

$$a_M^{(I)\dagger} = (-)^{2I} \tilde{a}_M^{[I]} = (-)^{I+M} \tilde{a}_{-M}^{(I)} \quad (5a)$$

$$\tilde{a}_M^{[I]\dagger} = (-)^{2I} a_M^{(I)} = (-)^{I-M} a_{-M}^{[I]} \quad (5b)$$

With these definitions there holds for any quantity:  $A^{\dagger\dagger} = A$ . The equations (3)-(5) are valid even if the  $a_M^{(I)\dagger}$ ,  $a_M^{(I)}$  are creation and annihilation operators, i.e., if the problem is treated in the occupation number formalism. If they are simply c-number amplitudes, then there holds

$$a_M^{(I)\dagger} = a_M^{(I)*} \quad (6a)$$

which can be used together with eq. (4) and (5) to define all amplitudes. Finally, for some quantities, e.g.,  $\gamma_m^{[\lambda]} =: (-i)^\lambda \gamma_{\lambda m}$ , there holds

$$\tilde{A}_M^{[I]} = A_M^{[I]} \quad (6b)$$

Such quantities are called "self conjugate."

With our conventions, the conjugation (3) becomes

$$\psi^\dagger = \sum_M (-)^{2I} \tilde{a}_M^{[I]} \tilde{\psi}_M^{(I)} = \hat{I} [\tilde{a}^{[I]} \tilde{\psi}^{[I]}] [0] \quad (3')$$

We now are prepared to introduce the irreducible density matrices, which we shall write as  $\rho_M^{[L]}$ . They are defined in the reduction of the direct product  $\psi^\dagger \psi$  into components of good angular momentum. We achieve this by recoupling (see Fig. 1), to obtain

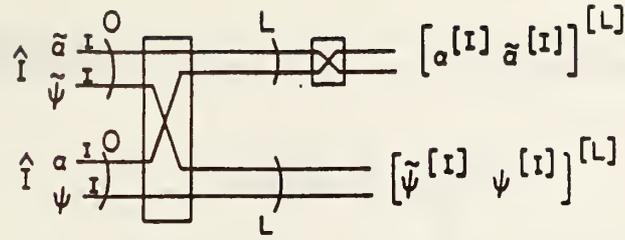


Figure 1

$$\begin{aligned}
 \psi^\dagger \psi &= \hat{I}^2 [\tilde{a}^{[I]} \tilde{\psi}^{[I]}]_{[0]} [a^{[I]} \psi^{[I]}]_{[0]} \\
 &= \sum_L \hat{I}^2 \begin{bmatrix} I & I & 0 \\ I & I & 0 \\ L & L & 0 \end{bmatrix} [[\tilde{a}^{[I]} a^{[I]}]_{[L]} [\tilde{\psi}^{[I]} \psi^{[I]}]_{[L]}]_{[0]} \\
 &= \sum_L \hat{I}^2 (-)^{2I-L} [\rho^{[L]} [\tilde{\psi}^{[I]} \psi^{[I]}]_{[L]}]_{[0]} . \quad (7)
 \end{aligned}$$

Here we have introduced the irreducible density matrix  $\rho^{[L]}$  by the definition

$$\rho_m^{[L]} =: [a^{[I]} \tilde{a}^{[I]}]_{[L]} . \quad (8)$$

Below we will give a justification for the choice of the coupling order.

Before continuing we would like to remark that particular caution must be paid if the amplitudes  $a^{[I]}$  are in fact annihilation-creation operators. So, for example, if one is dealing with a many-body system and if one writes out the operator  $a^{[I]}$  explicitly in terms of single-particle operators, e.g., for a two-body system

$$a_M^{[I]} = [\alpha^{[j]} \beta^{[k]}]_M^{[I]} \quad (9)$$

one has, in view of

$$(\alpha\beta)^\dagger = \beta^\dagger \alpha^\dagger \quad (10)$$

for the adjoint operator  $\tilde{a}_M^{[I]}$ , i.e., the creation operator, the order

$$\tilde{a}_M^{[I]} = (-)^{j+k-I} [\tilde{\beta}^{[k]} \tilde{\alpha}^{[j]}]_M^{[I]} . \quad (11)$$

More generally, in the case of a many-body system, e.g.,

$$A_M^{[I]} = [[[\alpha^{[j]} \beta^{[k]}]^{[I_1]} \gamma^{[\ell]}]^{[I_2]} \dots]_M^{[I]} \quad (12)$$

one has for the adjoint operator

$$\tilde{A}_M^{[I]} = (-)^{j+k+\ell+\dots-I} [\dots [\gamma^{[\ell]} [\tilde{\beta}^{[k]} \tilde{\alpha}^{[j]}]^{[I_1]}]^{[I_2]}]_M^{[I]} . \quad (13)$$

The phase factor is recognized as the usual phase factor associated with the re-ordering of the coupling. It is independent of the details of the coupling scheme, i.e., of the intermediate angular momenta  $I_1, I_2$ , etc. The same phase factor applies also if the particles occupy identical orbits, i.e., if  $j = k = \ell$ , etc. It then is  $(-)^{Nj-I}$  for  $N$  particles in the  $j$  shell. At any rate, usually it is not advantageous to employ the occupation number representation when one works with coupled operators as, for example, with eq. (12), but it is easier to achieve the required symmetry of the wave functions by means of a fractional parentage expansion. A detailed discussion of this subject is contained in Ref. 5.

We now can evaluate the mean value of an operator for the state (4).

Take an operator of multipolarity  $K$ :

$$\Omega =: \sum_k \omega_k^{(K)} \Omega_k^{[K]} = \hat{K} [\omega^{[K]} \Omega^{[K]}]^{[0]} . \quad (14)$$

Then we have, according to Fig. 2

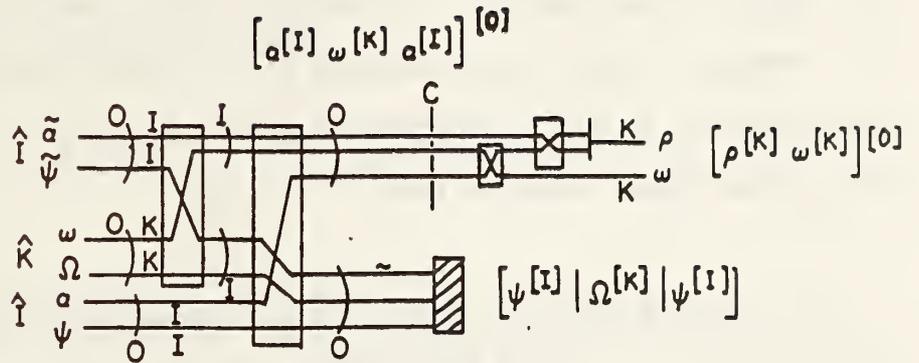


Figure 2

$$\begin{aligned}
 \langle \hat{\psi} | \Omega | \hat{\psi} \rangle &= \sum \hat{I}^2 \hat{K} \begin{bmatrix} I & I & 0 \\ K & K & 0 \\ I & I & 0 \end{bmatrix} \begin{bmatrix} I & I & 0 \\ I & I & 0 \\ 0 & 0 & 0 \end{bmatrix} (-)^{I+K-I} (-)^{I+I-K} \\
 &\times [\hat{\psi}^{[I]} | \Omega^{[K]} | \hat{\psi}^{[I]}] [\hat{a}^{[I]} \hat{a}^{[I]} \omega^{[K]}]^{[0]} \\
 &= (-)^{2I} [\hat{\rho}^{[K]} \omega^{[K]}]^{[0]} [\hat{\psi}^{[I]} | \Omega^{[K]} | \hat{\psi}^{[I]}] . \quad (15)
 \end{aligned}$$

The structure of (15) displays the well-known obvious facts: (i) in order to yield a finite expectation value the system must have a density matrix which has a non-vanishing component of the required multipolarity; in other words, only one multipolarity of the density matrix contributes to the expectation value. (ii) the orientations of the operator (given by the set  $\omega_k^{(K)}$ ) and of the system (specified by the set  $\rho_k^{[K]}$ ) must match; in other words, the expectation value is proportional to the quantity  $[\rho^{[K]} \omega^{[K]}]^{[0]}$ , which is the generalization to arbitrary  $K$  of the usual scalar product of vector algebra, where  $K = 1$ .

The phase  $(-)^{2I}$  in eq. (15) arises since the density matrix incorporates a reordering transformation. To see this more clearly, consider the general case for pure states, i.e., the case of a transition matrix element, say, for the transition  $\psi_I \rightarrow \psi_L$ . Changing in Fig. 2  $\tilde{\psi}_I$  to  $\tilde{\psi}_L$ , i.e., changing I to L in the top two input lines, we have

$$\begin{aligned}
 \langle \psi_L | \Omega | \psi_I \rangle &= \hat{I} \hat{K} \hat{L} \begin{bmatrix} L & L & 0 \\ K & K & 0 \\ I & I & 0 \end{bmatrix} \begin{bmatrix} I & I & 0 \\ I & I & 0 \\ 0 & 0 & 0 \end{bmatrix} [\tilde{a}^{[I]} \omega^{[K]} a^{[L]}]^{[0]} [\psi^{[L]} | \Omega^{[K]} | \psi^{[I]}] \\
 &= [\tilde{a}^{[L]} \omega^{[K]} a^{[I]}]^{[0]} [\psi^{[L]} | \Omega^{[K]} | \psi^{[I]}] \quad (16) \\
 &= (-)^{K+I-L} (-)^{I+L-K} [a^{[L]} \tilde{a}^{[I]} \omega^{[K]}]^{[0]} [\psi^{[L]} | \Omega^{[K]} | \psi^{[I]}] \quad (16a)
 \end{aligned}$$

The step from (16) to (16a) represents the re-ordering shown in Fig. 2 after the dashed line C.

For an impure state one cannot factorize the amplitudes and one must bring the state amplitudes together in order to achieve a density matrix. One actually has two choices for defining the density matrix, the choice (8), employed in Fig. 2, and the opposite order, exchanging  $a$  and  $\tilde{a}$ . In that case the second crossing in Fig. 2 would be absent, and the phase  $(-)^{2I}$  of (15) would be replaced by  $(-)^K$ . Clearly, the first choice is preferable: independently of the multipolarity of the operator and the density matrix, the introduction of a density matrix for a half-integer system yields a minus sign, i.e., the value of the crossing boxes of Fig. 2.

The structure of eq. (8) suggests the definition of the reducible density matrix:

$$\bar{\rho}_{mm'} =: a_m^{[I]} \tilde{a}_{m'}^{[I]} \quad (17)$$

This matrix is fully contra-standard. The coupling to good angular momentum, i.e., the construction of an irreducible density matrix, is performed using the normal vector coupling coefficients:

$$\rho^{[L]} = \sum_{mm'} (Im \ Im' | LM) \bar{\rho}_{mm'} \quad . \quad (18)$$

A more general case arises in the context of the evaluation of a transition probability. Formally it arises by writing for the operator (14) the direct product

$$\Omega = | T^\dagger | f \rangle \langle f | T | \quad . \quad (19)$$

The operator T can be a single multipole or, as in a plane wave, a mixture of multipoles. This way (15) then yields the square of the transition matrix element:

$$\langle \psi_i | T^\dagger | \psi_f \rangle \langle \psi_f | T | \psi_i \rangle = |M|^2 \quad , \quad (20)$$

which is directly the transition probability, of course, except for the kinematical factors. Writing

$$T =: \sum_K \hat{K} [t^{[K]} T^{[K]}] [0] \quad (21)$$

we obtain for (21) from Fig. 3



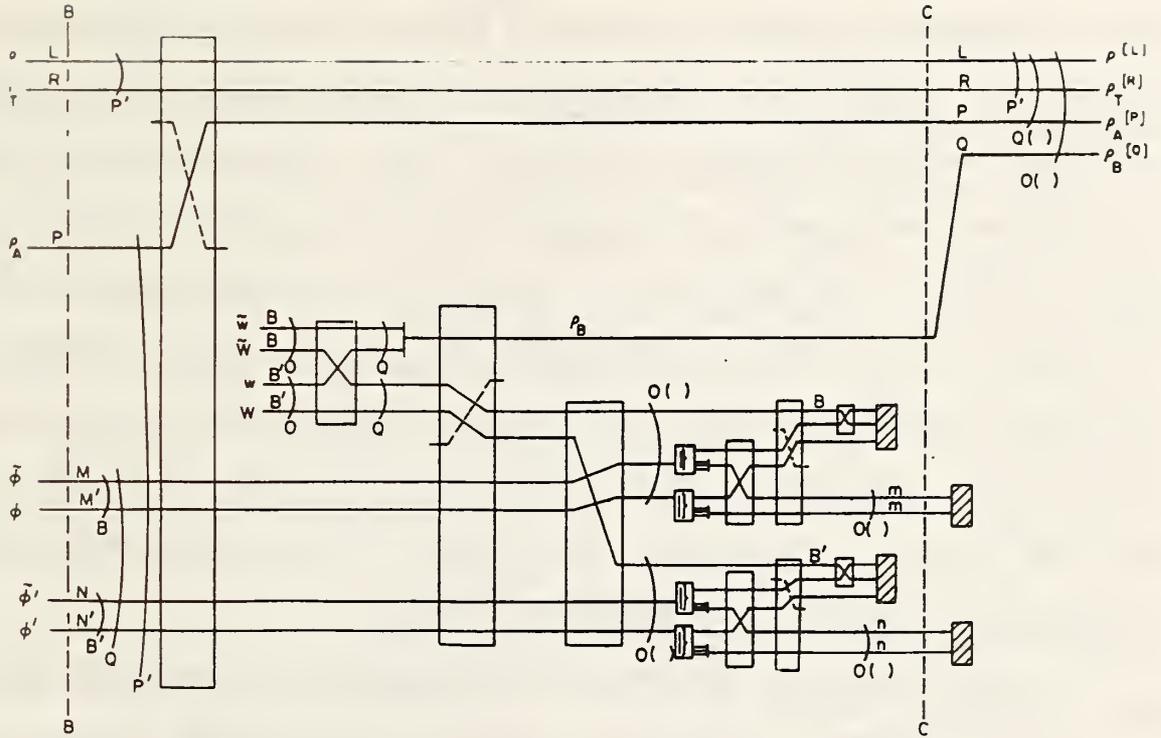


Figure 5

$$\begin{aligned}
 |M|^2 = & \sum_{KK'L} \hat{L}^2 \hat{I}^2 \hat{K} \hat{K}' \begin{bmatrix} I & I & 0 \\ I & I & 0 \\ L & L & 0 \end{bmatrix} \begin{bmatrix} K & K & 0 \\ K' & K' & 0 \\ L & L & 0 \end{bmatrix} \begin{bmatrix} J & J & 0 \\ J & J & 0 \\ 0 & 0 & 0 \end{bmatrix} \frac{1}{\hat{J}} \begin{bmatrix} L & L & 0 \\ L & L & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} I & I & L \\ K & K' & L \\ J & J & 0 \end{bmatrix} \begin{bmatrix} J & J & 0 \\ J & J & 0 \\ 0 & 0 & 0 \end{bmatrix} (-)^{K+L-I} \\
 & \times [\rho^{[L]} \tilde{t}^{[K]} t^{[K']} ] [0] [\psi^{[I]} | \tilde{T}^{[K]} | \psi^{[J]} ] [\psi^{[J]} | T^{[K']} | \psi^{[I]} ] \quad (22a)
 \end{aligned}$$

$$\begin{aligned}
 = & \sum_{KK'L} (-)^{K+J+I} \frac{1}{\hat{J}^3} \begin{bmatrix} I & I & L \\ K & K' & L \\ J & J & 0 \end{bmatrix} [\psi^{[I]} | \tilde{T}^{[K]} | \psi^{[J]} ] [\psi^{[J]} | T^{[K']} | \psi^{[I]} ] \\
 & \times [\rho^{[L]} \tilde{t}^{[K]} t^{[K']} ] [0] \quad . \quad (22b)
 \end{aligned}$$

For self-conjugate transition operators one may omit the tildas in (22b). In the case where the operator consists of a single multipole, the sum over  $K, K'$  collapses into a single term. Note that the final form (22b) still contains a recoupling coefficient (here, a 6-j type). This is the consequence of the fact that the density matrix ties together the matrix elements  $M$  and  $M^*$ , as evident from (8): the amplitude  $a$  originates in  $M$ , the amplitude  $\tilde{a}$  in  $M^*$ . The recoupling coefficient in (22b) unties the invariant matrix elements. It thus seems that for pure states, the use of the density matrix only introduces an unnecessary complication. But even for pure states the use of the amplitude rather than the density matrix allows for no simplification when analyzing the final state, as demonstrated below.

In equation (22) the information of the particular experimental set-up, i.e., the preparation of the initial state, etc. is contained in the invariant product  $[\rho^{[L]} \tilde{t}^{[K]} t^{[K]}]^{[0]}$ . Of course, here

$$[\tilde{t}^{[K]} t^{[K]}]^{[L]} := \rho_T^{[L]} \quad (23a)$$

are the density matrices characterizing the transition operator.

To obtain the characteristics of the complete reaction, e.g., the angular correlations in  $(\gamma, p)$  or  $(\gamma, p, n)$  reactions, etc., one simply continues the graph by inserting an appropriate analysis section. We illustrate this by the case of the emission of one particle. The analysis section here is inserted in the region shown by the dashed line A-A in Fig. 3. In its place we insert the graph shown in Fig. 4, which also shows the line A-A, beyond which lies the original graph of Fig. 3. The operator which analyzes the, say, angular distribution, or polarization, etc., of the emitted particle is  $[\omega\Omega]$ ; it provides the density matrix  $\rho_A^{[P]}$ ,

$$\rho_A^{[P]} =: \sum_{A,A'} [\tilde{\omega}^{[A']} \omega^{[A]}]^{[P]} . \quad (23b)$$

We here have allowed for the general case that the analyzing operator is given by a mixture of multipoles. The angular momentum P replaces some zeroes in the earlier coupling graph, Fig. 3. Therefore, some quantum numbers of Fig. 3 are not fixed and are to be replaced by the quantum numbers given in the first parentheses; in general they must be summed over their respective range of allowed values. For example, the density matrices  $\rho$  and  $\rho_T$  instead of being coupled to zero are coupled to P, and hence the density matrix  $\rho_T$  does not have to have multipolarity L; consequently L here is replaced by R. In Fig. 4 we also notice the symbols for the fractional parentage coefficients (or, more generally, the spectroscopic factors), which break the A-body system into a one-body plus an (A-1) - body system. The angular distribution (and/or polarization) of the emitted particle (labelled j) is analyzed by the operator  $\Omega$ , the orientation of which is described by the density matrix  $\rho_A$ . The angular distribution etc., is given by the quantity  $[\rho^{[L]} \rho_T^{[R]} \rho_A^{[P]}]^{[0]}$ , of course, summed over all values of L, R, P, contained in the experimental situation. We shall not bother to write out the algebraic expression of Fig. 4. Of course, the complete expression is the product of the expressions of Fig. 3 and Fig. 4.

We now continue the analysis to the case of the sequential emission of a second particle. To that end one continues the graph by replacing the region B-B of Fig. 4 by the graph of Fig. 5. Consequently some quantum numbers of Fig. 3 and Fig. 4 must be generalized, as indicated in the drawing; in Fig. 4 by the quantum numbers in the parentheses and in Fig. 3 by the quantum numbers in the second parentheses. The essential point is that the wave functions of

the (A-1) system are not terminated in overlap matrix elements but further decomposed into a one-body and an (A-2)-body system. The one-body part is analyzed by the operator  $W$ , and the (A-2)-body system is overlapped away. The details of this part of the problem have been discussed in Ref. 4, and even more extensively in Chapter 6 of Ref. 5. Clearly this procedure can be continued to achieve the complete description of reactions resulting in the emission of arbitrarily many particles, by cutting the graph at C-C and in essence repeating the procedure of Fig. 5. In other words, the procedure of going from  $n$  detected reaction products to  $n + 1$  detected reaction products is the same as that going from one to two detected particles, shown in Fig. 5.

The density matrices here arrive in the "natural" coupling scheme, i.e.,  $[[[\rho \rho_T \rho_A \rho_B \dots]]^{[0]}$ . This may not be the desired form; for example, one may be interested in the correlation between the two emitted particles. Then one would re-couple the density matrices as  $[[\rho \rho_T][\rho_A \rho_B \dots]]^{[0]}$ . In the extreme case where one is interested only in the correlation, one would put  $L = T = 0$ , i.e., ignore the unnecessary information. Or, one wants only the total cross section. Then one restricts the summation to the terms  $P = Q = 0$ ; analogously for any other situation. We here shall not go into further details, as our aim was only to demonstrate the use of the irreducible density matrices, and the ease of arriving at the final results without any problems in phasing, in particular in the interference terms which here arise automatically in the form of the summation over the angular quantum numbers allowed by triangularity and contained in the experimental setup.

### III. IMPURE STATES

If the system is not in a pure state, it cannot be described by a wave function. In that case, in essence one must start with Fig. 2. The density matrices  $\rho^{[K]}$  then must be given directly. The system is still defined by eq. (7), except that the left hand side of (7) has only symbolic meaning.

This way we arrive at the following rule of working with density matrices for impure systems. One may begin with the output side of Fig. 2, i.e., with the right-hand side of eq. (16). However, in case of doubt, make a graph for the case of pure states. Then introduce the permutation in the invariant triple product of the amplitudes as in Fig. 2, and replace the "pure" density matrix  $[a^{[I]} \tilde{a}^{[I]}]^{[K]}$  by the density matrix  $\rho^{[K]}$  describing the actual system. That means, that from now on for impure systems  $\rho^{[K]}$  must be treated as a single tensor. Otherwise all usual rules of writing down the algebraic expressions for the recoupling diagram remain unchanged. In particular, the central recoupling graph rule holds: write down the product of all symbols appearing in the graph, including all crossing phases. Precisely for this reason it is inadvisable to incorporate the phase  $(-)^{2I}$  of eq. (15) into the definition of the density matrix, even though the eq. (15) then would look simpler in that it would have no explicit phase. However, then the central rule of using recoupling graphs would be broken.

As an example for an impure system consider a cryogenic alignment experiment. A nucleus interacts at temperature  $T$  with the crystalline field. Let us assume that this field is given by a mixture of multipoles. The Hamiltonian then can be written

$$H = \sum_K \hat{K} [h^{[K]} H^{[K]}]^{[0]} \quad . \quad (24)$$

We first determine the eigenstates of the Hamiltonian, which of necessity are pure states. Thus, writing

$$H \Psi_n = E_n \Psi_n \quad (25)$$

and, if  $I$  is the spin of the nucleus,

$$\Psi_n = \hat{I} [S_n^{[I]} \psi^{[I]}] [0] \quad (26)$$

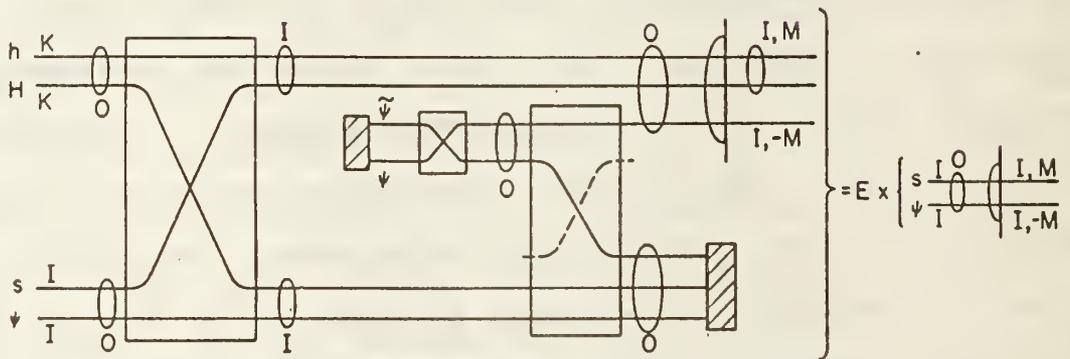


Figure.6

we have (see Fig. 6)

$$\begin{aligned} & \sum_{MK} \hat{K} \hat{I} \begin{bmatrix} K & K & 0 \\ I & I & 0 \\ I & I & 0 \end{bmatrix} \hat{I} (-)^{2I} \begin{bmatrix} I & I & 0 \\ 0 & I & I \\ I & 0 & I \end{bmatrix} [\psi^{[I]} | H^{[K]} | \psi^{[I]}] \\ & \times (IM | -M | 00) [h^{[K]} S_n^{[I]}]_M^{[I]} \psi_{-M}^{[I]} \\ & = \sum_M E_n (IM | -M | 00) S_{nM}^{[I]} \psi_{-M}^{[I]} \quad (27) \end{aligned}$$

Equating the coefficients of  $\psi_{-M}^{[I]}$  and evaluating the recoupling coefficients we obtain

$$\sum_{KKM'} [\psi_{-M}^{[I]} | H^{[K]} | \psi_{-M}^{[I]}] (KkIM' | IM) h_k^{[K]} S_{nM'}^{[I]} = E_n S_{nM}^{[I]} \quad (28)$$

which is the eigenvalue equation for  $\psi_n$ . Using

$$\hat{S}_{nM}^{[I]} = (-)^{I-M} S_{n-M}^{[I]*}$$

one can construct the density matrix for the pure states  $\psi_n$ :

$$\bar{\sigma}_{nMM'} = S_{nM}^{[I]} \hat{S}_{nM'}^{[I]} \quad (29)$$

The density matrix for the target nucleus at equilibrium with the target crystal at temperature  $T = 1/\beta$  is given by

$$\bar{\rho}_{MM'} = Z^{-1} \sum_n e^{-\beta E_n} \bar{\sigma}_{nMM'} \quad (30)$$

$$Z = \sum_n e^{-\beta E_n} .$$

One sees that, indeed,  $\bar{\rho}_{MM'}$  cannot be factorized. It can only be written as a sum of factorizable matrices.

The irreducible density matrices are again constructed by eq. (18). They are handled exactly as the irreducible density matrices for pure states.

Of course, one encounters cases where the system is not in a state of definite angular momentum. The most prominent of such cases is a scattering state where the incoming particle is a plane wave. No difficulties arise in this case, as has been already discussed above. The independent summation over the different multipoles ( $K, K', A, A',$  etc.) yields directly the interferences between the different multipoles; there is no difference between the cases of the pure and the impure states, when the expressions are written in terms of the density matrices.

#### IV. RELATION TO THE USUAL DEFINITIONS

The density matrix usually is defined by

$$\rho_{mm'} = a_m^{(I)} a_{m'}^{(I)*} = (-)^{2I} a_m^{(I)} \tilde{a}_{m'}^{[I]} \quad (31)$$

and the state is given by

$$\rho_{mm'} = \psi_m^{[I]} \tilde{\psi}_{m'}^{(I)} \quad (32)$$

The mean value of a component of an operator then is

$$\begin{aligned} \langle \Omega_k^{[K]} \rangle &= \text{Tr } \rho \Omega \\ &= \sum_{mm'} \rho_{mm'} \langle \psi_{m'}^{[I]} | \Omega_k^{[K]} | \psi_m^{[I]} \rangle \quad (33) \end{aligned}$$

Here both the matrix elements and the density matrix are mixed quantities in both gender and angular momentum. We have,

$$\rho_{mm'} = (-)^{I-m} \bar{\rho}_{-mm'} \quad (34)$$

and thus the reduction in angular momentum is

$$\rho_M^{[L]} = \sum (I-m \ I m' | LM) (-)^{I-m} \rho_{mm'} \quad (35)$$

which is not the familiar form for coupling angular momenta. When using density matrices, it is therefore advisable to work exclusively with  $\bar{\rho}$ . As demonstrated above with the example of the polarized target it is always possible to obtain directly the fully contrastandard  $\bar{\rho}$ . There thus is no need to introduce at all the mixed gender  $\rho$ . At any rate, if one has  $\rho$  available one can construct  $\bar{\rho}$  by means of (34).

## APPENDIX

For the convenience of the reader we list here some symbols. More details are given in Chapter 4 of Ref. 5.

### 1. Definition of invariant matrix element

$$\int \psi_{m_1}^{[j_1]+} T_k^{[K]} \psi_{m_2}^{[j_2]} := (-)^{j_1+m_1} (-)^{j_1-K+j_2} \begin{pmatrix} j_1 & K & j_2 \\ -m_1 & k & m_2 \end{pmatrix} [\psi^{[j_1]} | T^{[K]} | \psi^{[j_2]}]. \quad (A1)$$

### 2. Relation between the invariant matrix element and the reduced matrix element

$$\langle \psi^{[j_1]} | T^{[K]} | \psi^{[j_2]} \rangle = (-)^{j_1+K-j_2} [\psi^{[j_1]} | T^{[K]} | \psi^{[j_2]}]. \quad (A2)$$

### 3. Special case $T^{[K]} = 1$ : overlap

$$[\psi^{[I]} | 1 | \psi^{[I]}] =: [\psi^{[I]} | \psi^{[I]}] = \hat{I}. \quad (A3)$$

### 4. Amplitude overlap

$$[a^{[I]} | a^{[I]}] = 1/\hat{I} \quad (A4)$$

### 5. 9j - type recoupling coefficient

$$\begin{bmatrix} a & b & c \\ d & e & f \\ g & h & i \end{bmatrix} =: \hat{c}\hat{f}\hat{g}\hat{h} \left\{ \begin{matrix} a & b & c \\ d & e & f \\ g & h & i \end{matrix} \right\}. \quad (A5)$$

## REFERENCES

1. U. Fano, Rev. Mod. Phys. 29, 74 (1957).
2. U. Fano and G. Racah, Irreducible Tensorial Sets, Academic Press, New York (1959).
3. M. Danos, Ann. Phys. (N.Y.) 63, 319 (1971).
4. M. Danos and V. Gillet, Relativistic Many-Body Bound Systems, NBS Monograph 147 (1975).
5. M. Danos, V. Gillet, and M. Cauvin, Methods in Relativistic Nuclear Physics, North Holland (Amsterdam, Oxford, New York, Tokyo) (1984).

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